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1 Recipes for adjoint code construction

Ralf Giering, Thomas Kaminski

December 1998 **ACM Transactions on Mathematical Software (TOMS)**, Volume 24 Issue 4

Full text available: pdf(301.79 KB) Additional Information: full citation, abstract, references, citings, index terms

Adjoint models are increasingly being developed for use in meteorology and oceanography. Typical applications are data assimilation, model tuning, sensitivity analysis, and determination of singular vectors. The adjoint model computes the gradient of a cost function with respect to control variables. Generation of adjoint code may be seen as the special case of differentiation of algorithms in reverse mode, where the dependent function is a scalar. The described method for adjoint code gene ...

Keywords: adjoint model, adjoint operator, automatic differentiation, computational differentiation, data assimilation, differentiation of algorithms, implicit functions, inverse modeling, optimization, reverse mode

2 Demonstrating the scalability of a molecular dynamics application on a Petaflop computer

George S. Almasi, Călin Caşcaval, José G. Castaños, Monty Denneau, Wilm Donath, Maria Eleftheriou, Mark Giampapa, Howard Ho, Derek Lieber, José E. Moreira, Dennis Newns, Marc Snir, Henry S. Warren

June 2001 **Proceedings of the 15th international conference on Supercomputing**

Full text available: pdf(392.72 KB) Additional Information: full citation, abstract, references, citings, index terms

The IBM Blue Gene project has endeavored into the development of a cellular architecture computer with millions of concurrent threads of execution. One of the major challenges of this project is demonstrating that applications can successfully exploit this massive amount of parallelism. Starting from the sequential version of a well known molecular dynamics code, we developed a new application that exploits the multiple levels of parallelism in the Blue Gene cellular architecture. We perform ...

Keywords: Blue Gene, cellular architecture, massively parallel computing, molecular dynamics, performance evaluation

3 Symbolic-numeric stability investigations of Jameson's schemes for the thin-layer Navier-Stokes equations

V. G. Ganzha, E. V. Vorozhtsov, J. Boers, J. A. van Hulzen

August 1994 **Proceedings of the international symposium on Symbolic and algebraic computation**

Full text available: pdf(790.89 KB) Additional Information: full citation, abstract, references, index terms

The Navier-Stokes equations governing the three-dimensional flows of viscous, compressible, heat-conducting gas and augmented by turbulence modeling present the most realistic model for gas flows around the elements of aircraft configurations. We study the stability of one of the Jameson's schemes of 1981, which approximates the set of five Navier-Stokes equations completed by the turbulence model of Baldwin and Lomax. The analysis procedure implements the check-up of the necessary von Neum ...

4 PELLPACK: a problem-solving environment for PDE-based applications on multicomputer platforms

E. N. Houstis, J. R. Rice, S. Weerawarana, A. C. Catlin, P. Papachiou, K.-Y. Wang, M. Gaitatzes

March 1998 **ACM Transactions on Mathematical Software (TOMS)**, Volume 24 Issue 1

Full text available: pdf(26.30 MB) Additional Information: full citation, abstract, references, citings, index terms, review

The article presents the software architecture and implementation of the problem-solving environment (PSE) PELLPACK for modeling physical objects described by partial differential equations (PDEs). The scope of this PSE is broad, as PELLPACK incorporates many PDE solving systems, and some of these, in turn, include several specific PDE solving methods. Its coverage for 1D, 2D. and 3D elliptic or parabolic problems is quite broad, and it handles some hyperbolic problems, Since a PSE should p ...

Keywords: PDE language, execution models, knowledge bases, libraries, parallel reuse methodologies, problem-solving environments, programming-in-the-large, sofeware bus

5 Session P8: nature visualization: Visualizing dynamic molecular conformations

Johannes Schmidt-Ehrenberg, Daniel Baum, Hans Christian Hege

October 2002 **Proceedings of the conference on Visualization '02**

Full text available: pdf(2.72 MB) Additional Information: full citation, abstract, references, index terms

The bioactivity of a molecule strongly depends on its metastable conformational shapes and the transitions between these. Therefore, conformation analysis and visualization is a basic prerequisite for the understanding of biochemical processes.We present techniques for visual analysis of metastable molecular conformations. Core of these are flexibly applicable methods for alignment of molecular geometries, as well as methods for depicting shape and 'fuzziness' of metastable conformations. All an ...

Keywords: drug design, molecular conformation analysis, molecular modeling, uncertainty visualization

6 An analytic approach to significance assessment in local sequence alignment with gaps

R. Bundschuh

April 2000 **Proceedings of the fourth annual international conference on Computational molecular biology**

Full text available: pdf(974.15 KB) Additional Information: full citation, abstract, references, citings

A detailed study of the Smith-Waterman alignment algorithm is performed in order to find an analytical approach to the problem of assessing the statistical significance of local alignments with gaps. The significance is shown to be given in terms of an eigenvalue equation which captures the dynamics of the much simpler global alignment algorithm. This eigenvalue equation is then explicitly solved for a simple scoring system and the resulting significance estimations are verified by a comparis ...

Keywords: Gumbel distribution, sequence alignment, statistical significance

7 Dynamic NURBS with geometric constraints for interactive sculpting

Demetri Terzopoulos, Hong Qin

April 1994 **ACM Transactions on Graphics (TOG)**, Volume 13 Issue 2

Full text available: pdf(8.87 MB) Additional Information: full citation, abstract, references, citings, index terms, review

This article develops a dynamic generalization of the nonuniform rational B-spline (NURBS) model. NURBS have become a defacto standard in commercial modeling systems because of their power to represent free-form shapes as well as common analytic shapes. To date, however, they have been viewed as purely geometric primitives that require the user to manually adjust multiple control points and associated weights in order to design shapes. Dynamic NURBS, or D-NURBS, are physics-based models tha ...

Keywords: CAGD, NURBS, constraints, cross-sectional shape design, deformable models, dynamics, finite elements, free-form deformation, optimal curve and surface fitting, shape metamorphosis, solid rounding, trimming

8 On design principles for a molecular computer

Michael Conrad

May 1985 **Communications of the ACM**, Volume 28 Issue 5

Full text available: pdf(2.50 MB) Additional Information: full citation, abstract, references, citings, index terms, review

If the unique information-processing capabilities of protein enzymes could be adapted for computers, then evolvable, more efficient systems for such applications as pattern recognition and process control are in principle possible.

9 SIGSAM BULLETIN: Computer algebra in the life sciences

Michael P. Barnett

December 2002 **ACM SIGSAM Bulletin**, Volume 36 Issue 4

Full text available: pdf(240.15 KB) Additional Information: full citation, abstract, references

This note (1) provides references to recent work that applies computer algebra (CA) to the life sciences, (2) cites literature that explains the biological background of each application, (3) states the mathematical methods that are used, (4) mentions the benefits of CA, and (5) suggests some topics for future work.

10 Efficient synthesis of physically valid human motion

Anthony C. Fang, Nancy S. Pollard

July 2003 **ACM Transactions on Graphics (TOG)**, Volume 22 Issue 3

Full text available: pdf(1.83 MB) Additional Information: full citation, abstract, references, citings, index terms

Optimization is a promising way to generate new animations from a minimal amount of input data. Physically based optimization techniques, however, are difficult to scale to complex animated characters, in part because evaluating and differentiating physical quantities becomes prohibitively slow. Traditional approaches often require optimizing or constraining parameters involving joint torques; obtaining first derivatives for these parameters is generally an $O(D^2)$ process ...

Keywords: animation, physically based animation

11 An algorithm with linear complexity for interactive, physically-based modeling of large proteins

Mark C. Surles

July 1992 **ACM SIGGRAPH Computer Graphics , Proceedings of the 19th annual conference on Computer graphics and interactive techniques**, Volume 26 Issue 2

Full text available: pdf(1.76 MB) Additional Information: full citation, references, citings, index terms

Keywords: Lagrange multiplier method, constrain systems, molecular modeling

12 Accurate performance evaluation, modelling and prediction of a message passing simulation code based on middleware

Michela Taufer, Thomas Stricker

November 1998 **Proceedings of the 1998 ACM/IEEE conference on Supercomputing (CDROM)**

Full text available: html(85.30 KB) Additional Information: full citation, abstract, references, citings

In distributed and vectorized computing there is a large number of highly different supercomputing platforms an application could run on. Therefore most traditional parallel codes are ill equipped to collect data about their resource usage or their behavior at run time and the corresponding data are rarely published and few scientists attack the planning of an application and its platform systematically. As an improvement over the current state of the art, we propose an integrated approach to pe ...

Keywords: PVM, application design methods, computer architecture, molecular dynamics, parallelization tools and middleware, performance monitoring, scientific application codes

13 Analysis of an efficient algorithm for the hard-sphere problem

Alan T. Krantz

July 1996 **ACM Transactions on Modeling and Computer Simulation (TOMACS)**, Volume 6 Issue 3

Full text available: pdf(481.83 KB) Additional Information: full citation, abstract, references, citings, index terms, review

Many similar algorithms for performing simulations of hard-sphere have been presented. Among these algorithms are those designed by Rapaport (RAP), Lubachevsky (LUB), Krantz (HAD), and Marin (HYBRID). These algorithms exhibit a similar design in that they each use an O(logn) event queue which becomes the overwhelming bottleneck when simulating large systems. In this paper the design of HAD is presented and contrasted to RAP, LUB and HYBRID. Next, both an em ...

Keywords: algorithm, discrete simulation, hard-sphere, manybody problem

14 Algorithmic issues in modeling motion

Pankaj K. Agarwal, Leonidas J. Guibas, Herbert Edelsbrunner, Jeff Erickson, Michael Isard, Sariel Har-Peled, John Hershberger, Christian Jensen, Lydia Kavraki, Patrice Koehl, Ming Lin, Dinesh Manocha, Dimitris Metaxas, Brian Mirtich, David Mount, S. Muthukrishnan, Dinesh Pai, Elisha Sacks, Jack Snoeyink, Subhash Suri, Ouri Wolefson

December 2002 **ACM Computing Surveys (CSUR)**, Volume 34 Issue 4

Full text available: pdf(205.25 KB) Additional Information: full citation, abstract, references, citings, index terms

This article is a survey of research areas in which motion plays a pivotal role. The aim of the article is to review current approaches to modeling motion together with related data structures and algorithms, and to summarize the challenges that lie ahead in producing a more unified theory of motion representation that would be useful across several disciplines.

Keywords: Computational geometry, computer vision, mobile networks, modeling, molecular biology, motion modeling, physical simulation, robotoics, spatio-temporal databases

15 Dynamic load balancing for the simulation of granular materials

R. Knecht, G. A. Kohring

July 1995 **Proceedings of the 9th international conference on Supercomputing**

Full text available: pdf(562.78 KB) Additional Information: full citation, references, citings, index terms

16 TNPACK—a truncated Newton minimization package for large-scale problems: II. Implementation examples

Tamar Schlick, Aaron Fogelson

March 1992 **ACM Transactions on Mathematical Software (TOMS)**, Volume 18 Issue 1

Full text available: pdf(2.50 MB) Additional Information: full citation, references, citings, index terms

Keywords: nonlinear optimization, sparse matrices, truncated Newton methods

17 Dynamic smooth subdivision surfaces for data visualization

Chhandomay Mandal, Hong Qin, Baba C. Vemuri

October 1997 **Proceedings of the 8th conference on Visualization '97**

Full text available: pdf(1.13 MB) Publisher Site Additional Information: full citation, references, citings, index terms

Keywords: dynamics, finite elements, interactive techniques, subdivision surfaces, visualization

18 Fast methods for simulation of biomolecule electrostatics

Shihhsien S. Kuo, Michael D. Altman, Jaydeep P. Bardhan, Bruce Tidor, Jacob K. White

November 2002 **Proceedings of the 2002 IEEE/ACM international conference on Computer-aided design**

Full text available: pdf(338.15 KB) Additional Information: full citation, abstract, references, index terms

Computer simulation is an important tool for improving our understanding of biomolecule electrostatics, in part to aid in drug design. However, the numerical techniques used in these simulation tools do not exploit fast solver approaches widely used in analyzing integrated circuit interconnects. In this paper we describe one popular formulation used to analyze biomolecule electrostatics, present an integral formulation of the problem, and apply the precorrected-FFT method to accelerate the solut ...

19 Dynamics: Interactive physically based solid dynamics

M. Hauth, J. Groß, W. Straßer

July 2003 **Proceedings of the 2003 ACM SIGGRAPH/Eurographics Symposium on Computer animation**

Full text available: pdf(5.02 MB) Additional Information: full citation, abstract, references

The interactive simulation of deformable solids has become a major working area in Computer Graphics. We present a sophisticated material law, better suited for dynamical computations than the standard approaches. As an important example, it is employed to reproduce measured material data from biological soft tissue. We embed it into a state-of-the-art finite element setting employing an adaptive basis. For time integration the use of an explicit stabilized Runge-Kutta method is proposed.

20 Scalable atomistic simulation algorithms for materials research

Aiichiro Nakano, Rajiv K. Kalia, Priya Vashishta, Timothy J. Campbell, Shuji Ogata, Fuyuki Shimojo, Subhash Saini

November 2001 **Proceedings of the 2001 ACM/IEEE conference on Supercomputing (CDROM)**

Full text available: pdf(1.32 MB) Additional Information: full citation, abstract, references, citings, index terms

A suite of scalable atomistic simulation programs has been developed for materials research based on space-time multiresolution algorithms. Design and analysis of parallel algorithms are presented for molecular dynamics (MD) simulations and quantum-mechanical (QM) calculations based on the density functional theory. Performance tests have been carried out on 1,088-processor Cray T3E and 1,280-processor IBM SP3 computers. The linear-scaling algorithms have enabled 6.44-billion-atom MD and 111,000 ...

Keywords: data compression, density functional theory, load balancing, molecular dynamics, parallel computing, quantum mechanics, variable-charge molecular

dynamics

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The Journal of Chemical Physics -- October 15, 1997 -- Volume 107, Issue 15, pp. 5840-5851

Symplectic splitting methods for rigid body molecular dynamics

Andreas Dullweber
University Chemical Laboratories, Lensfield Road, Cambridge CB2 1EW, United Kingdom

Benedict Leimkuhler
Department of Mathematics, The University of Kansas, Lawrence, Kansas 66045

Robert McLachlan
Department of Mathematics, Massey University, Palmerston North, New Zealand

(Received 11 June 1997; accepted 15 July 1997)

Rigid body molecular models possess symplectic structure and time-reversal symmetry. Standard numerical integration met properties, introducing nonphysical dynamical behavior such as numerically induced dissipative states and drift in the energy simulations. This article describes the construction, implementation, and practical application of fast explicit symplectic-rever for multiple rigid body molecular simulations. These methods use a reduction to Euler equations for the free rigid body, toget symplectic splitting technique. In every time step, the orientational dynamics of each rigid body is integrated by a sequence Besides preserving the symplectic and reversible structures of the flow, this scheme accurately conserves the total angular m system of interacting rigid bodies. Excellent energy conservation can be obtained relative to traditional methods, especially i simulations. The method is implemented in a research code, ORIENT, and compared with a quaternion/extrapolation scher model of water. Our experiments show that the symplectic-reversible scheme is far superior to the more traditional quaternic *American Institute of Physics.*

PII: S0021-9606(97)02339-8
doi:10.1063/1.474310
PACS: 34.30.+h, 31.15.Qg, 33.20.Sn, 02.70.Ns, 02.30.Cj, 02.60.Jh Additional Information

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   Christopher J. Fennell *et al.*, J. Chem. Phys. **120**, 9175 (2004)
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   I. P. Omelyan *et al.*, Phys. Rev. E **66**, 026701 (2002)
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   Nobuyuki Matubayasi *et al.*, J. Chem. Phys. **114**, 4107 (2001)
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   Ramzi Kutteh *et al.*, Phys. Rev. E **61**, 3186 (2000)
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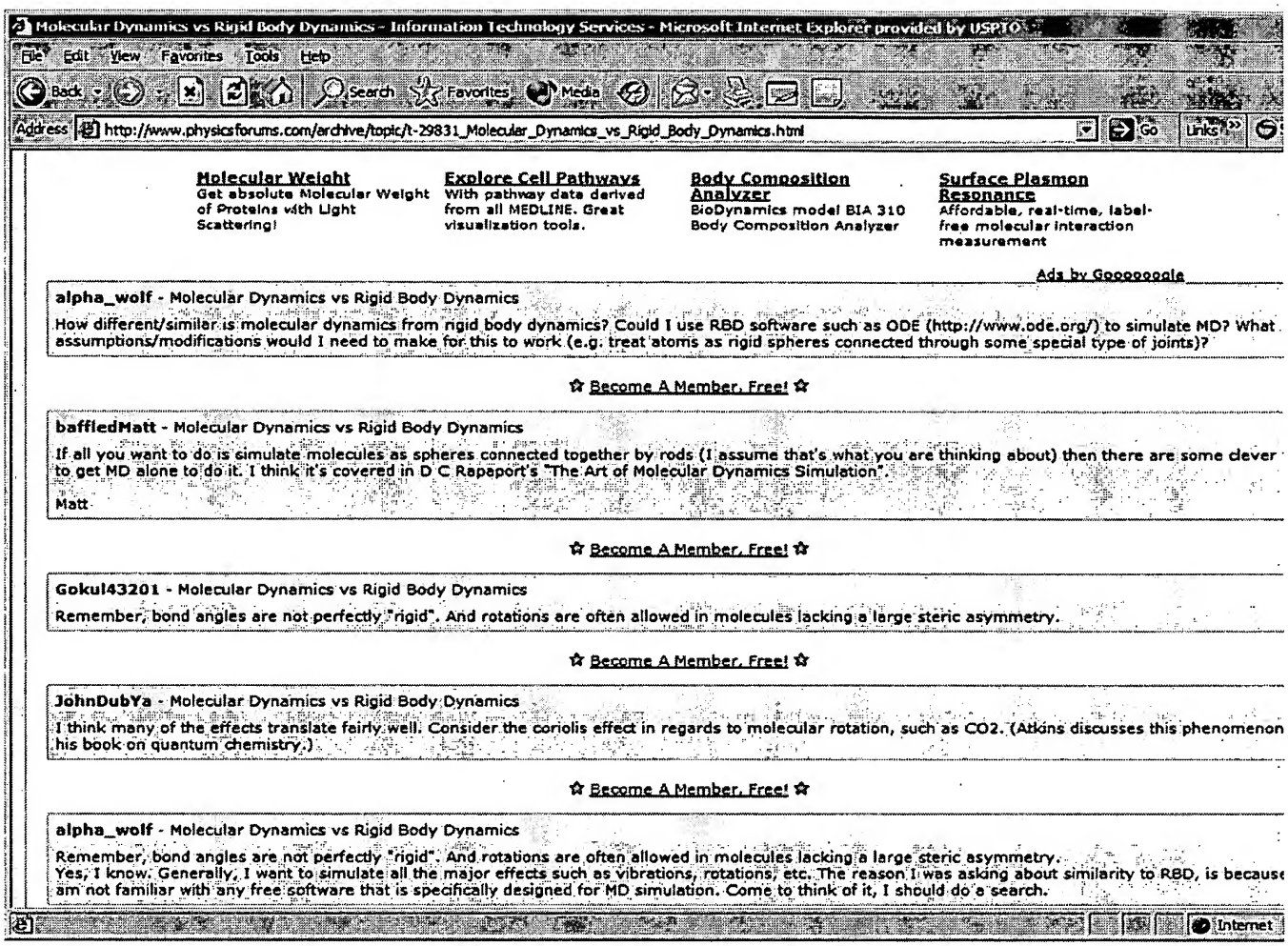
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How different/similar is molecular dynamics from rigid body dynamics? Could I use RBD software such as ODE (http://www.ode.org/) to simulate MD? What assumptions/modifications would I need to make for this to work (e.g. treat atoms as rigid spheres connected through some special type of joints)?
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baffledMatt - Molecular Dynamics vs Rigid Body Dynamics
If all you want to do is simulate molecules as spheres connected together by rods (I assume that's what you are thinking about) then there are some clever to get MD alone to do it. I think it's covered in D C Rapeport's "The Art of Molecular Dynamics Simulation".
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Remember, bond angles are not perfectly "rigid". And rotations are often allowed in molecules lacking a large steric asymmetry.
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JohnDubYa - Molecular Dynamics vs Rigid Body Dynamics
I think many of the effects translate fairly well. Consider the coriolis effect in regards to molecular rotation, such as CO2. (Atkins discusses this phenomenon his book on quantum chemistry.)
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Remember, bond angles are not perfectly "rigid". And rotations are often allowed in molecules lacking a large steric asymmetry.
Yes, I know. Generally, I want to simulate all the major effects such as vibrations, rotations, etc. The reason I was asking about similarity to RBD, is because am not familiar with any free software that is specifically designed for MD simulation. Come to think of it, I should do a search.
Internet

Note: Performing your original search, ***Virtual Rigid Body Dynamics***, in PubMed will retrieve *6* citations.

1: Biopolymers. 1991 Jan;31(1):77-100.

Virtual rigid body dynamics.

Head-Gordon T, Brooks CL 3rd.

Department of Chemistry, Carnegie-Mellon University, Pittsburgh, Pennsylvania 15213.

An important direction in biological simulations is the development of methods that permit the study of larger systems and/or longer simulation time scales than is currently feasible by molecular dynamics. One such method designed with this objective in mind is stochastic boundary molecular dynamics (SBMD). SBMD was developed for the characterization of spatially localized processes in proteins, and has been shown to successfully reproduce structural and dynamical properties of these macromolecules, as compared to a molecular dynamics control simulation, when concerted or global motions are not present. The virtual rigid body dynamics method presented in this work extends the range of applicability of the SBMD method, by providing a framework to include these important long time scale conformational transitions. In this paper we describe the two-step implementation of the virtual rigid body model: first, the reduction of the full atomic representation to a reduced particle (virtual bond) model, and second, the propagation of the dynamics of flexibly connected rigid bodies containing virtual atom sites.

MeSH Terms:

- Biopolymers
- Computer Simulation*
- Electrochemistry
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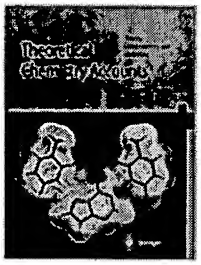

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Date: September 1998
Pages: 279 - 288

Recent advances in molecular dynamics simulation towards the realistic representation of biomolecules in solution

Thomas E. Cheatham III. [A1] and Bernard R. Brooks [A1]

[A1] Laboratory of Biophysical Chemistry, National Heart, Lung, and Blood Institute, 12A-2041, National Institutes of Health, 9000 Rockville Pike, Bethesda, MD 20892-5626, USA

Abstract:

Abstract. Coupled advances in empirical force fields and classical molecular dynamics simulation methodologies, combined with the availability of faster computers, has lead to significant progress towards accurately representing the structure and dynamics of biomolecular systems, such as proteins, nucleic acids, and lipids in their native environments. Thanks to these advances, simulation results are moving beyond merely evaluating force fields, displaying expected structural fluctuations, or demonstrating low root-mean-squared deviations from experimental structures and now provide believable structural insight into a variety of processes such as the stabilization of A-DNA in mixed water and ethanol solution or reversible #-peptide folding in methanol. The purpose of this overview is to take stock of these recent advances in biomolecular simulation and point out some common deficiencies exposed in longer simulations. The most significant methodological advances relate to the development of fast methods to properly treat long-range electrostatic interactions, and in this regard the fast Ewald methods are becoming the de facto standard.

Keywords:

Key words: Molecular dynamics · Biomolecular simulation

Head-Gordon, T. and Brooks, C.L. (1991). ``Virtual Rigid Body Dynamics", *Biopolymers* 31, 77--100.

T. E. Cheatham III and B. R. Brooks, "Recent Advances in Molecular Dynamics Simulation Towards Realistic Representation of Biomolecules in Solution," *Theoretical Chemistry Accounts* **99**, 279-288 (1998).

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